The Atomic-Scale Structure of Surfaces and Interfaces in III-V Semiconductor Devices

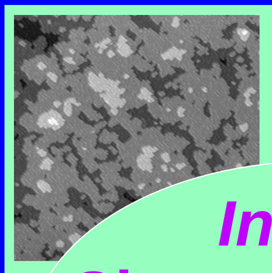
Lloyd J. Whitman, Naval Research Laboratory

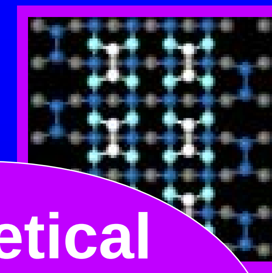
Third Workshop on the Fabrication, Characterization, and Applications of 6.1 Å III-V Semiconductors

August 2, 2001

Funded by ONR and DARPA-DSO

III-V Device Optimization





In-Situ
Characterization

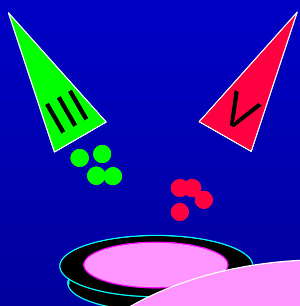
RHEED, XPS, STM

Theoretical Calculations

LDA, Modeling

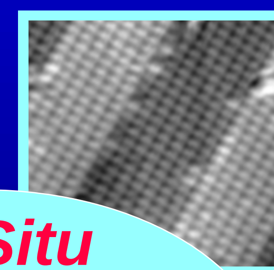
Device Performance

Electrical
Optical



MBE Growth

Temperature
Flux Rates
Interrupts



Ex-Situ
Characterization

X-STM X-ray
X-TEM Raman

Requires integrated approach.

Cast of Collaborators

From NRL:

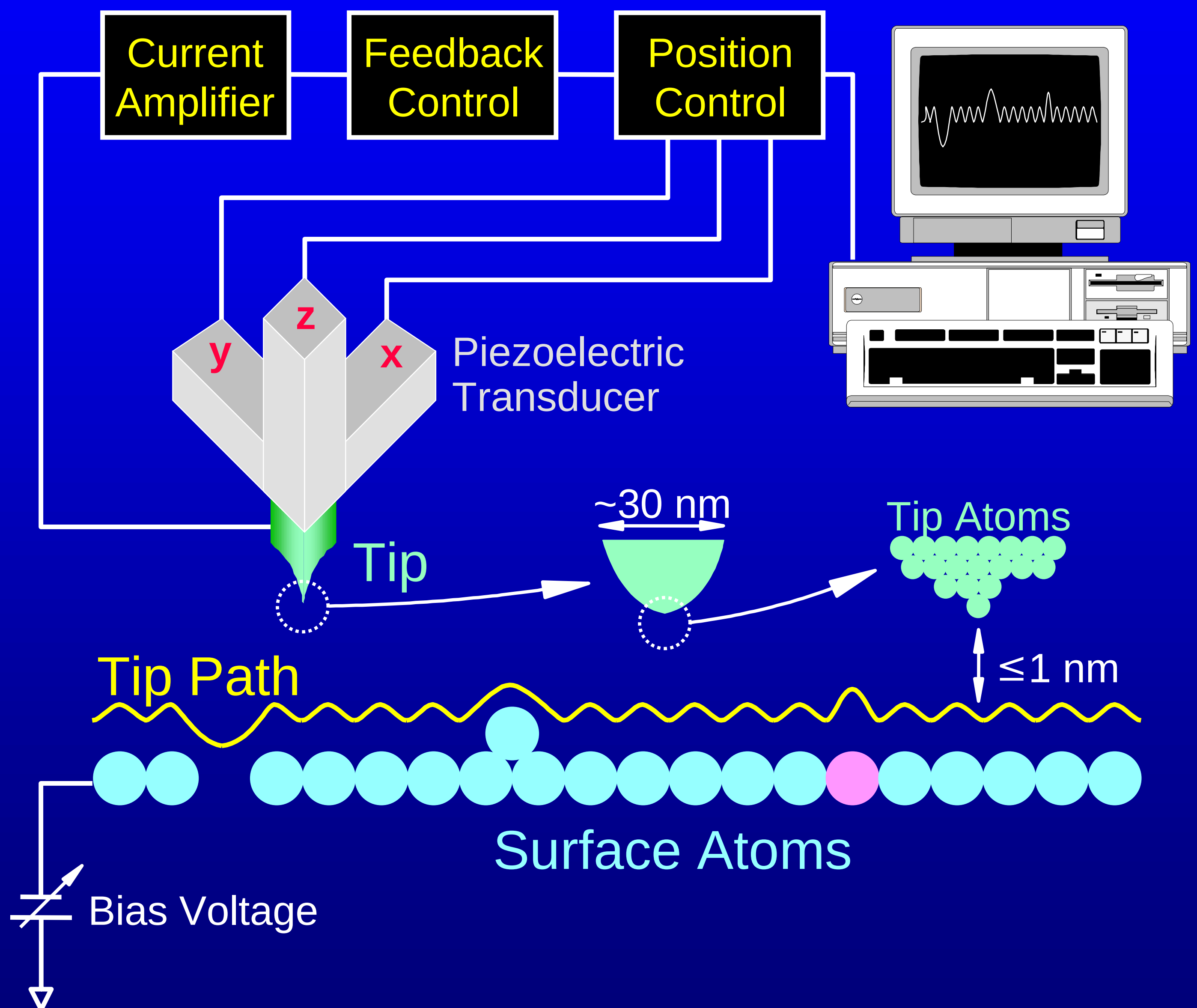
W. Barvosa-Carter → *HRL*
B. R. Bennett
A. S. Bracker
J. C. Culbertson
S. C. Erwin
S.-G. Kim → *.com*
R. Magno
B. Z. Nosho → *HRL*
B. V. Shanabrook
M. E. Twigg
M.-J. Yang

From Elsewhere:

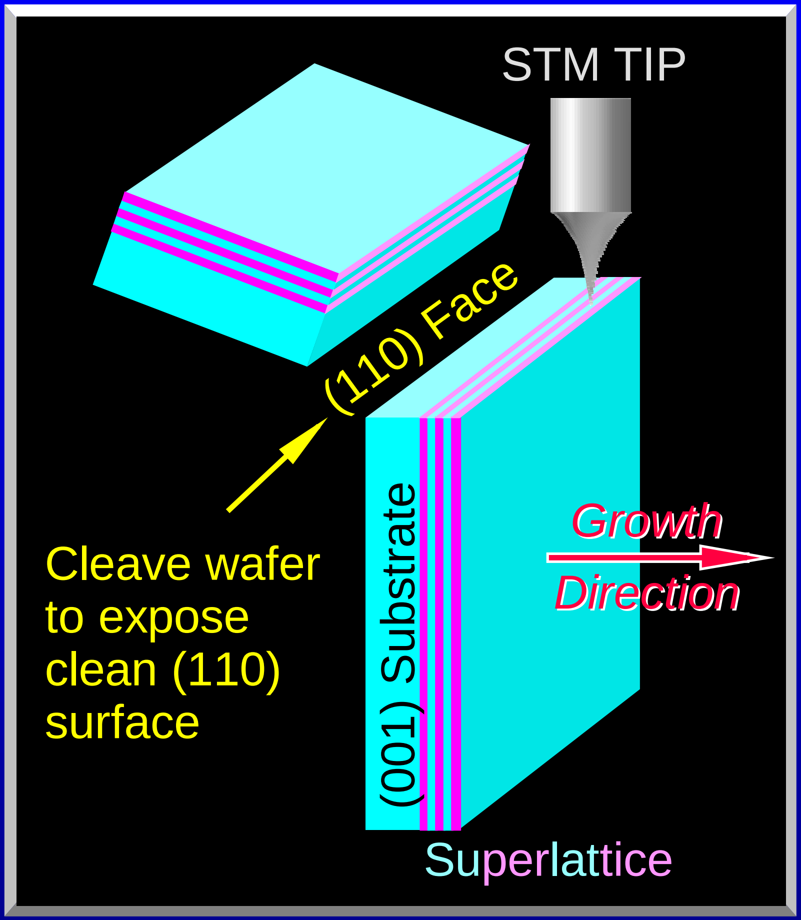
N. Modine, *Sandia*
H. Kim, E. Kaxiras, *Harvard*

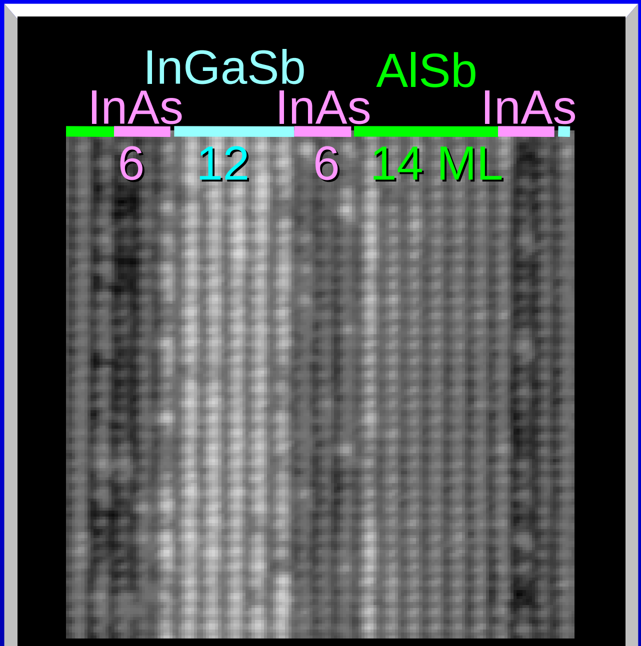
NRL Code 6000 Epicenter

Scanning Tunneling Microscopy



Cross-Sectional STM (X-STM)





X-STM of IR Laser

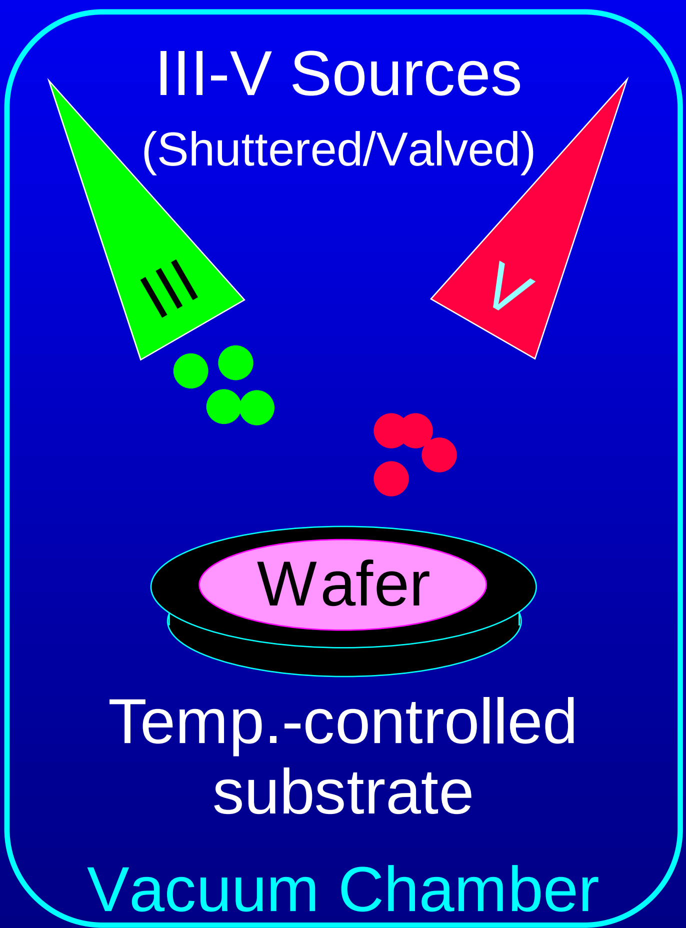
Major Issues

- Contrast: structural vs. electronic
- Quantifying interfacial roughnees

Combine experiments with first-principles theory.

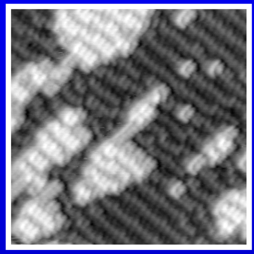
How Can Surface Characterization Help?

MBE

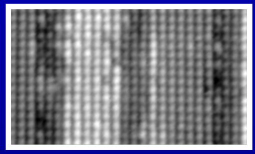


Monitor with RHEED

- Input for growth simulations, process control
  - Surface reconstructions, growth modes

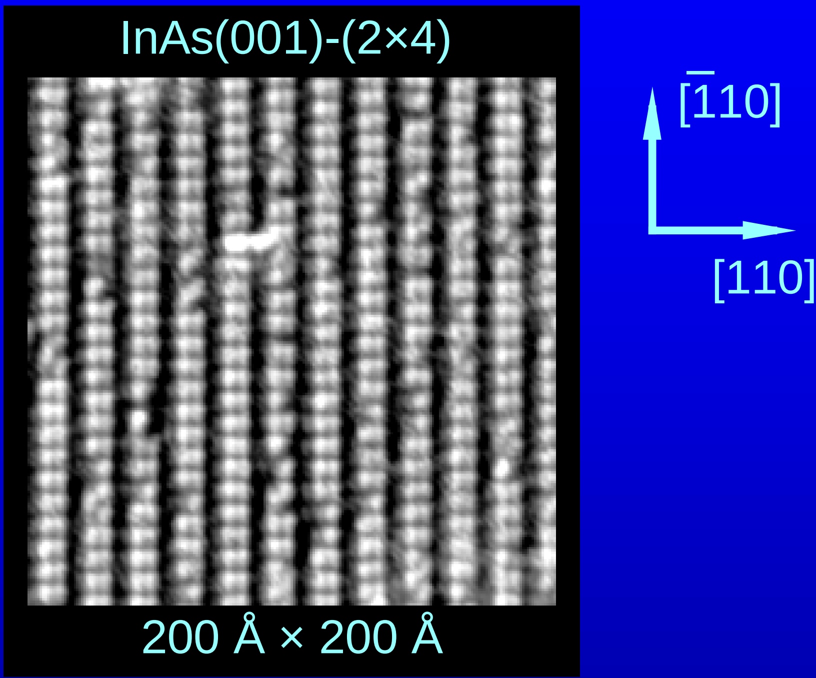


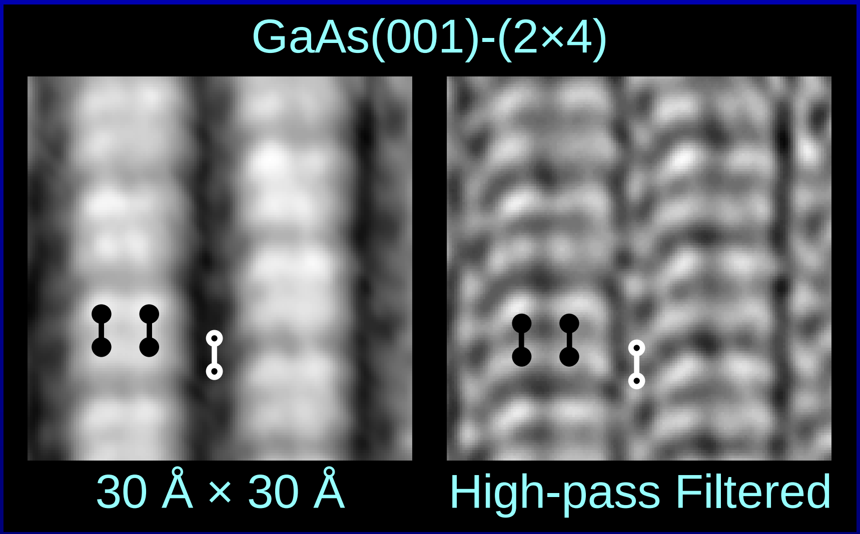
  - Correlate with in-situ probes
- Feedback to optimize growth
  - "Cook and look" -- analyze -- try again



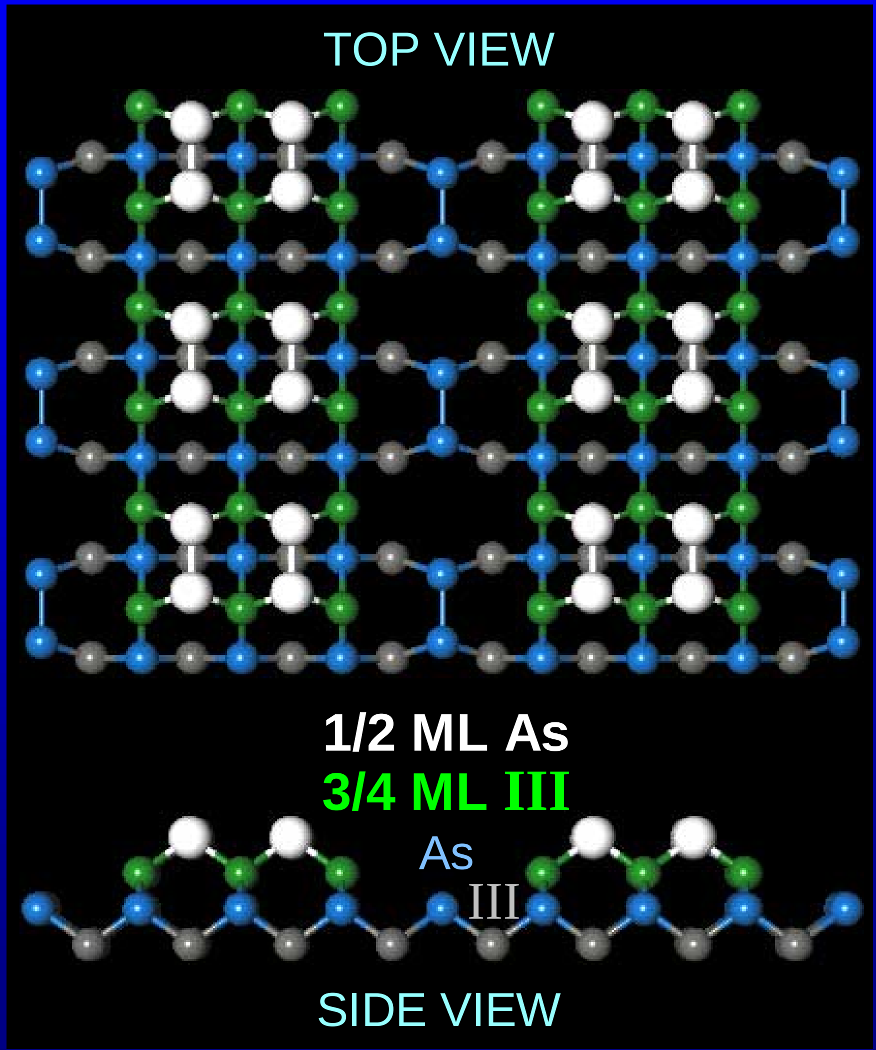
- Correlate surfaces/interfaces with electrical/optical prop.'s

III-As(001)-β2(2×4) Reconstruction



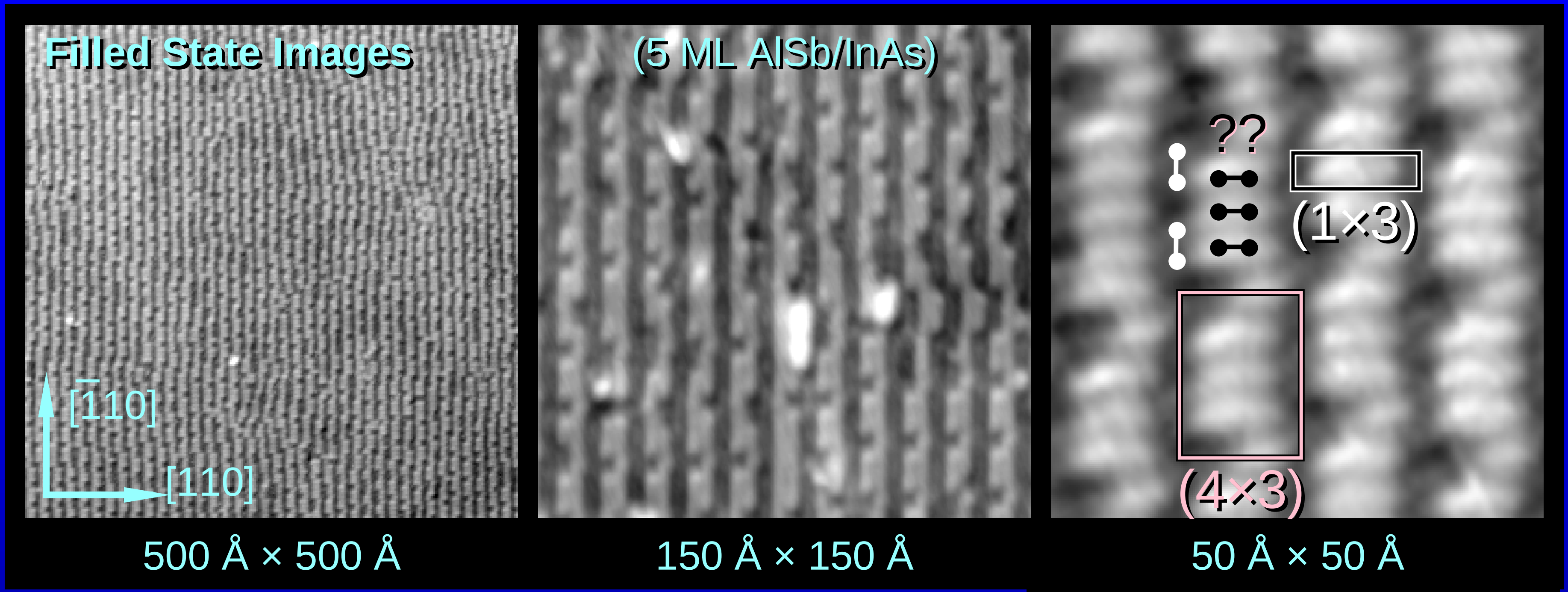


III-V(001)-β2(2×4)

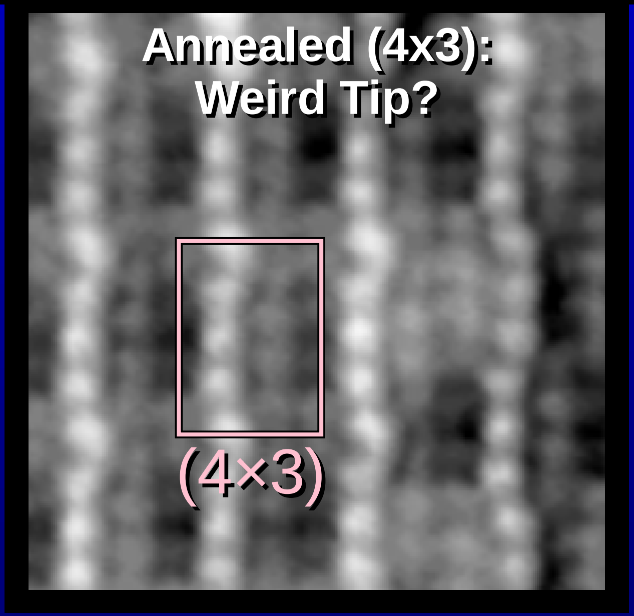


0.5 ML As on 0.75 ML III.

AlSb(001)-(1×3)-like Reconstruction

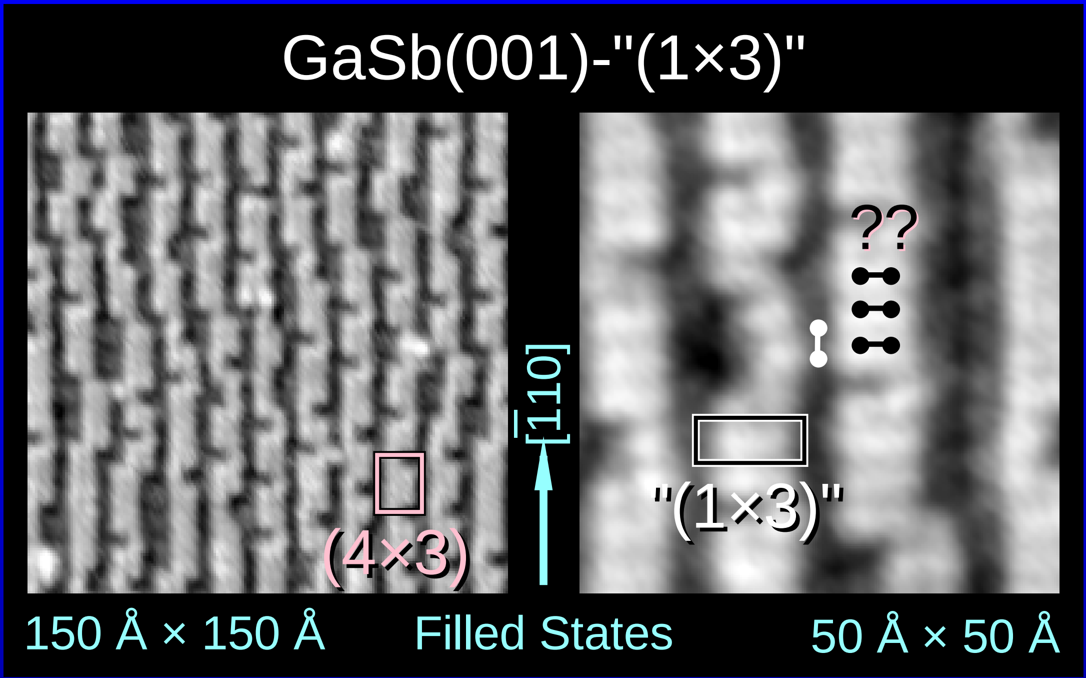


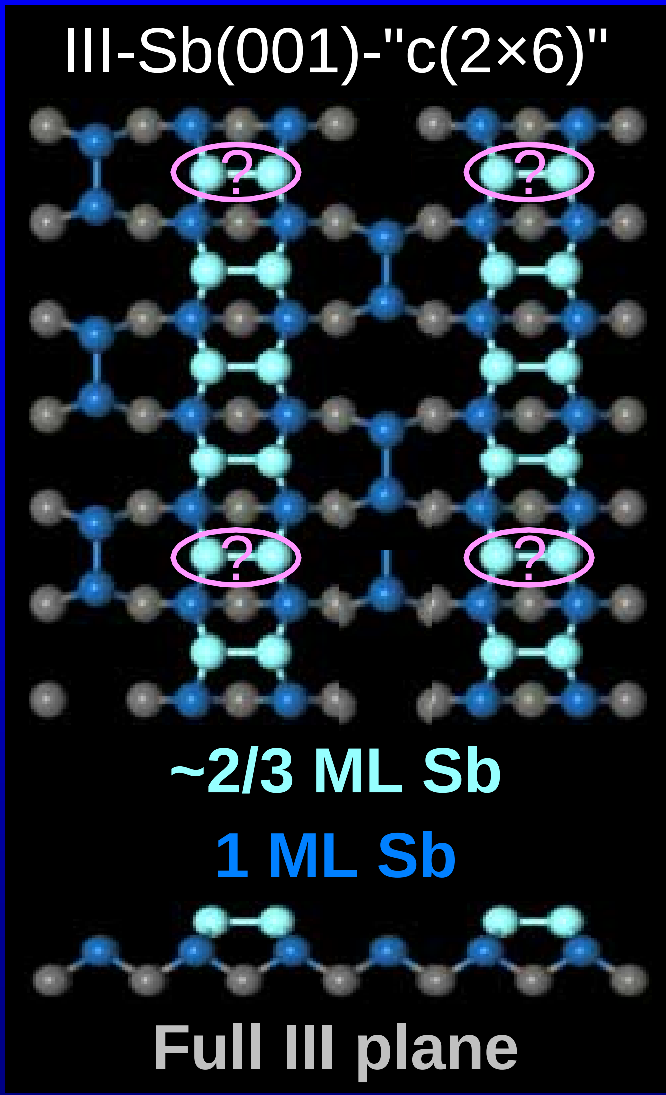
- RHEED typically "(1×3)" – depends strongly on *T*, Sb_4 flux
- At high T, low Sb_4, faint (4x3)



Quasi-periodic defects make local (4×3) domains.

III-Sb(001)-(1×3)-like Reconstructions



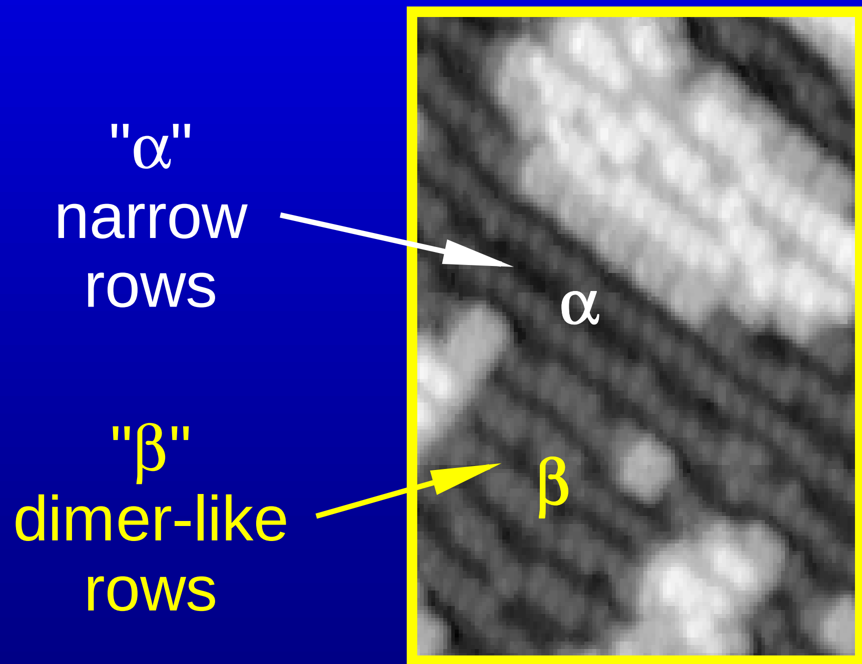


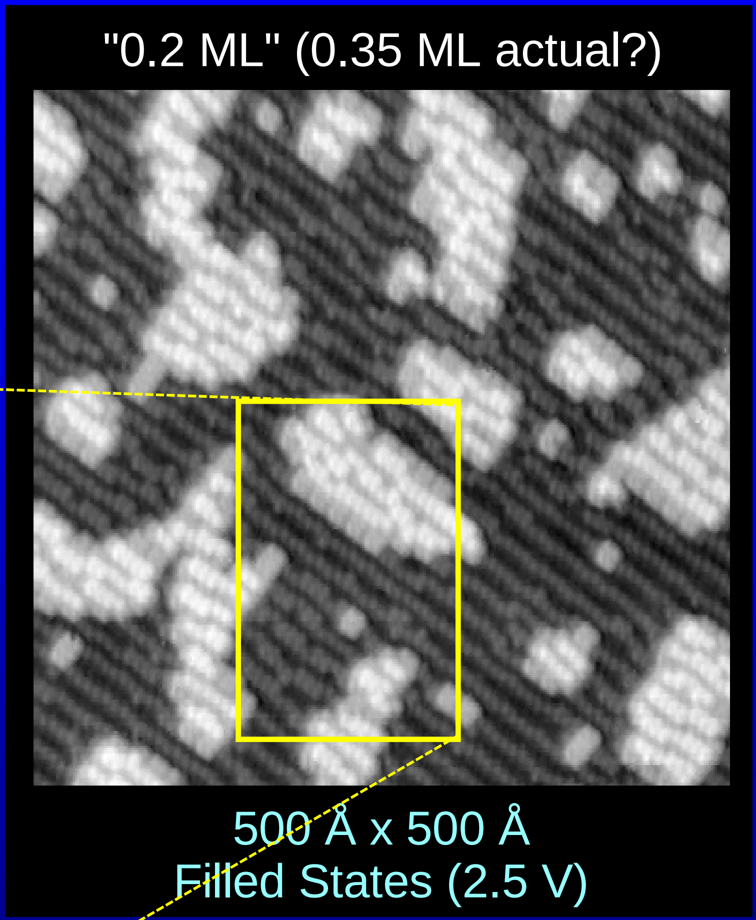
- (Al,Ga,In)Sb "(1×3)" all look similar
- Lowest energy structure is more complex (4×3) or (4×6)?

III-Sb(001)-"(1×3)" understood well enough?...

Initial Study of AlSb(001) Homoepitaxy

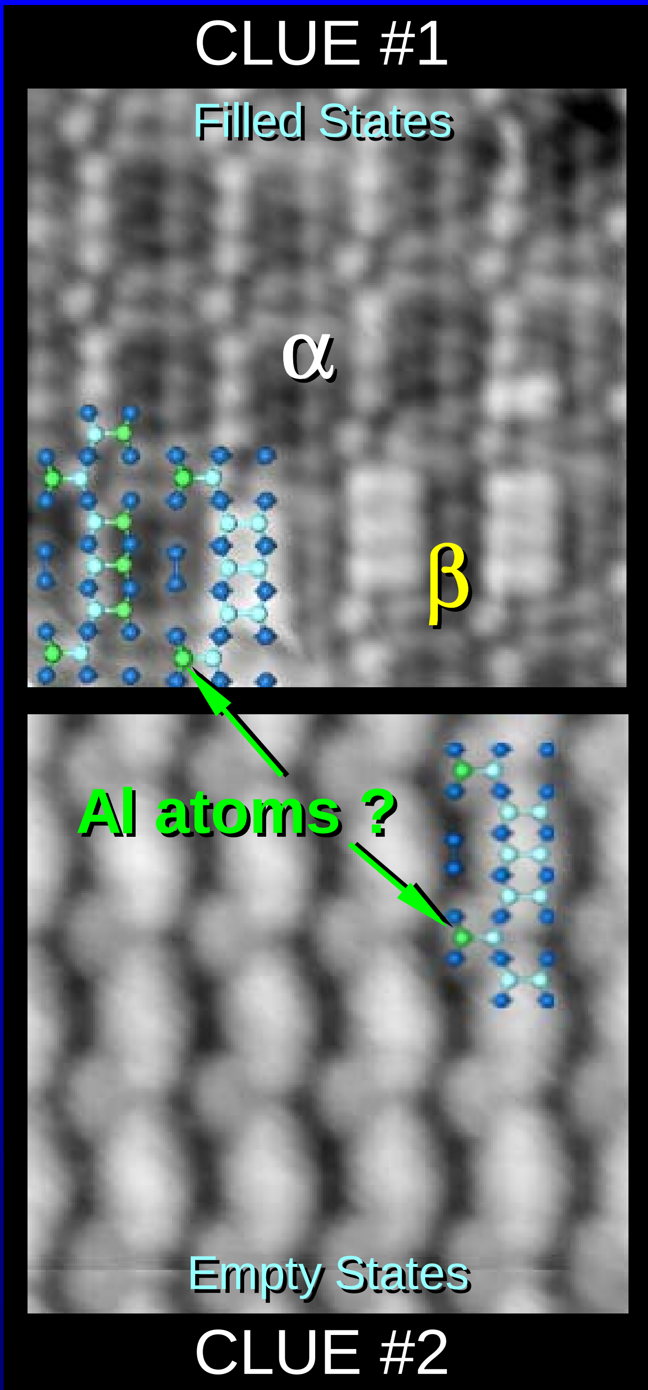
- Prepare "(1×3)," deposit 0.2 ML, **0.35 ML observed!**
- "(1×3)" actually *multiple* reconstructions



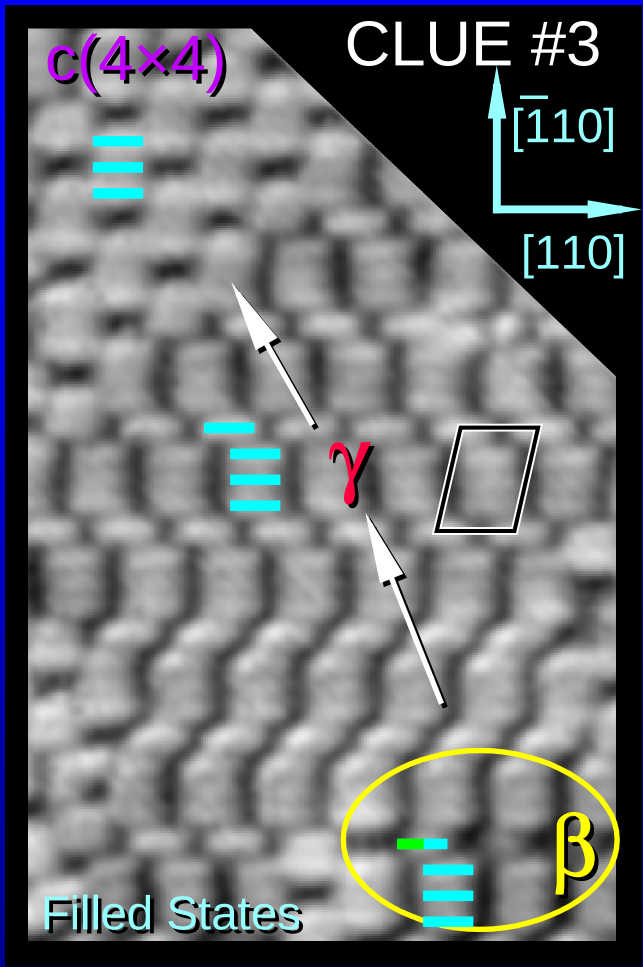


Something we don't understand about "(1×3)"...

The "(1×3)" Missing Links

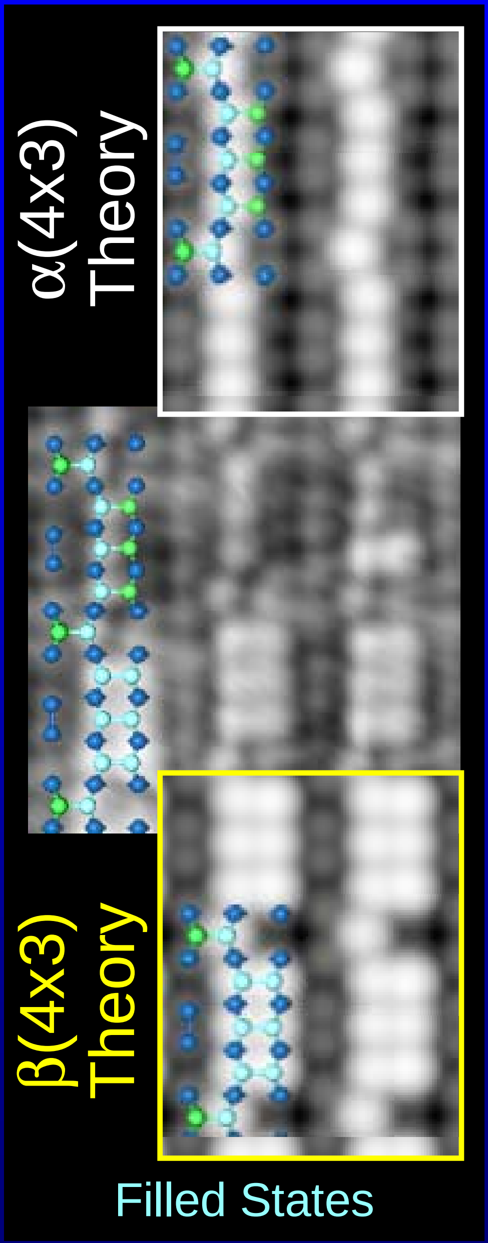


- Multiple (4×3) phases
- "Notch" is really a kink
- When more Sb rich, "notch" becomes Sb dimer kink



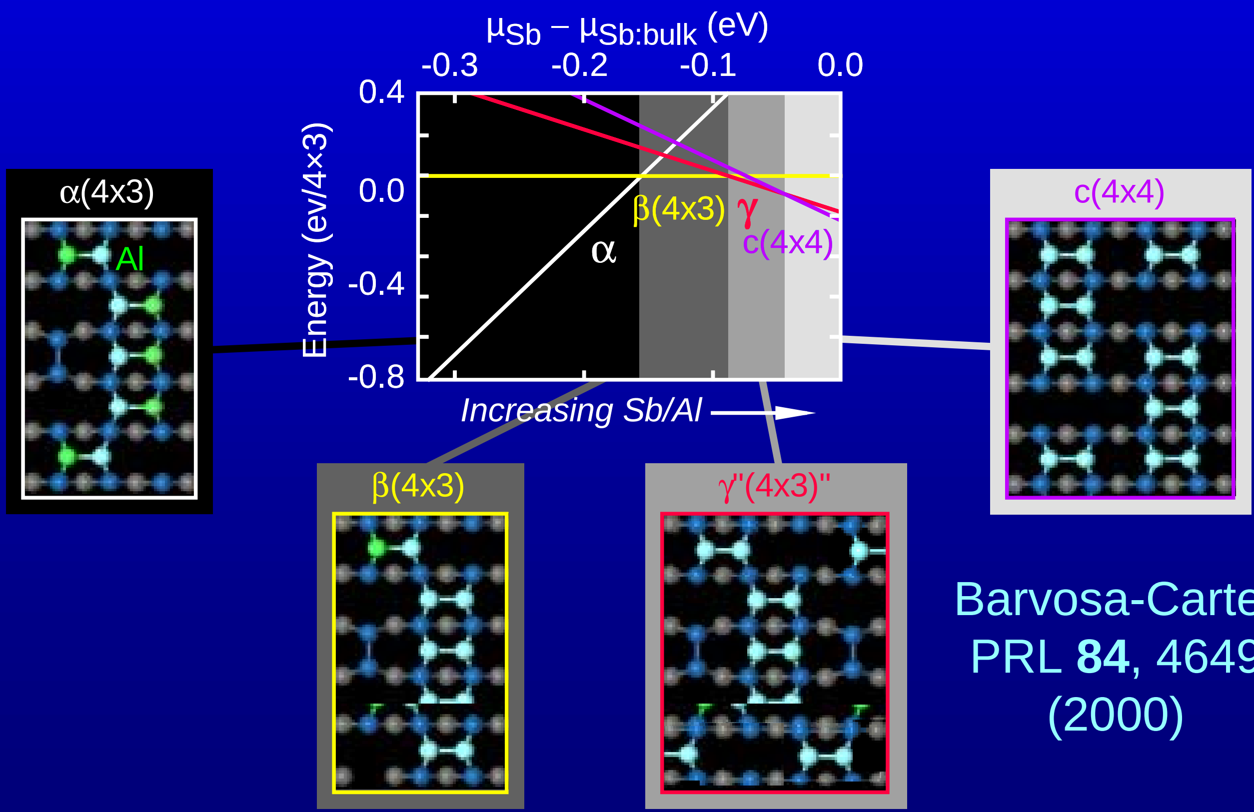
Multiple (4×3) structures, including novel mixed dimer?

AlSb Structures: Theory + Experiment



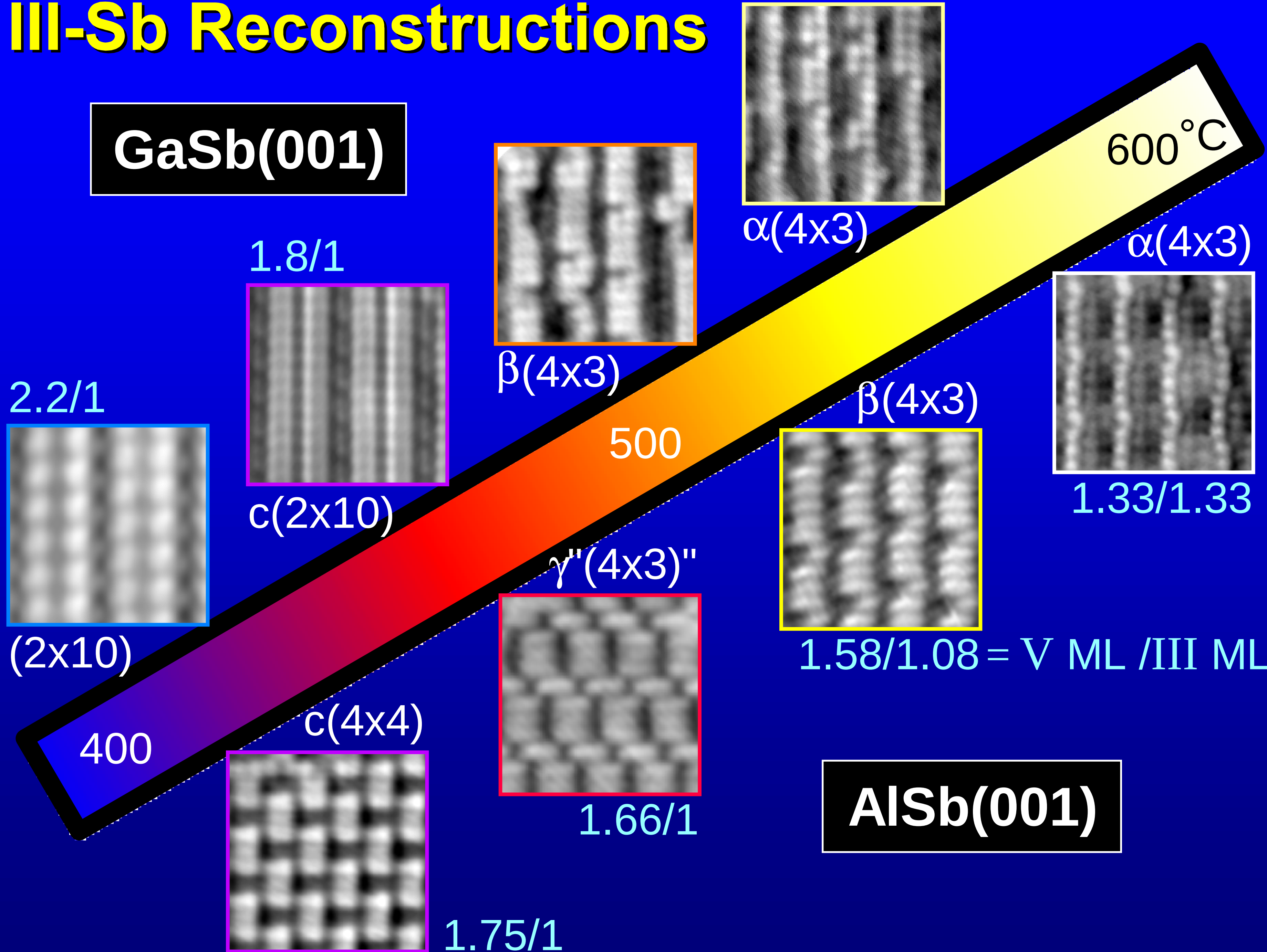
LDA by H. Kim, N. Modine, E. Kaxiras

- Novel Al+Sb mixed dimer in α and β(4×3) phases -- Al close to natural lattice site
- Theory: same relative stability vs. Sb flux

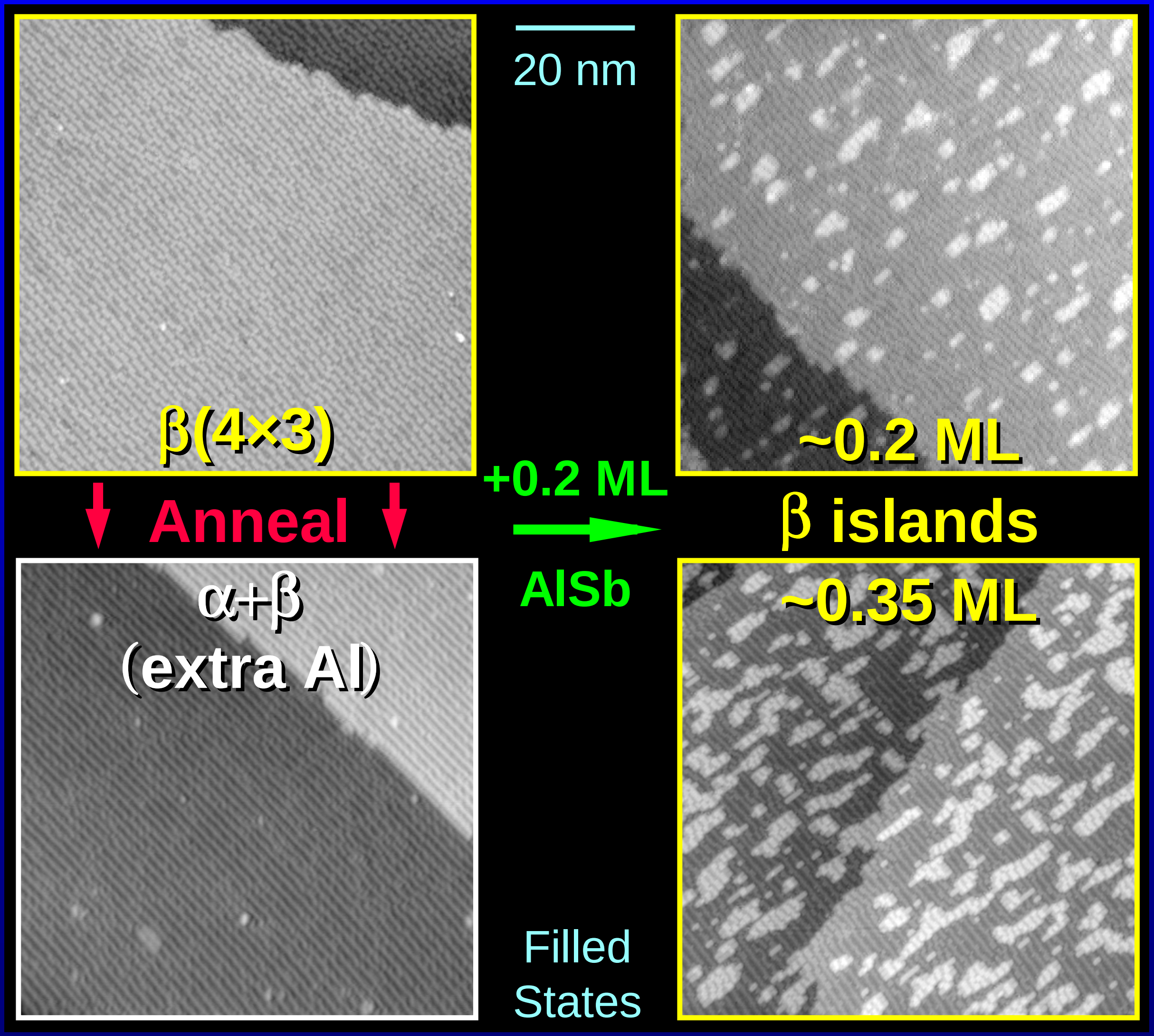


Barvosa-Carter
PRL **84**, 4649
(2000)

III-Sb Reconstructions



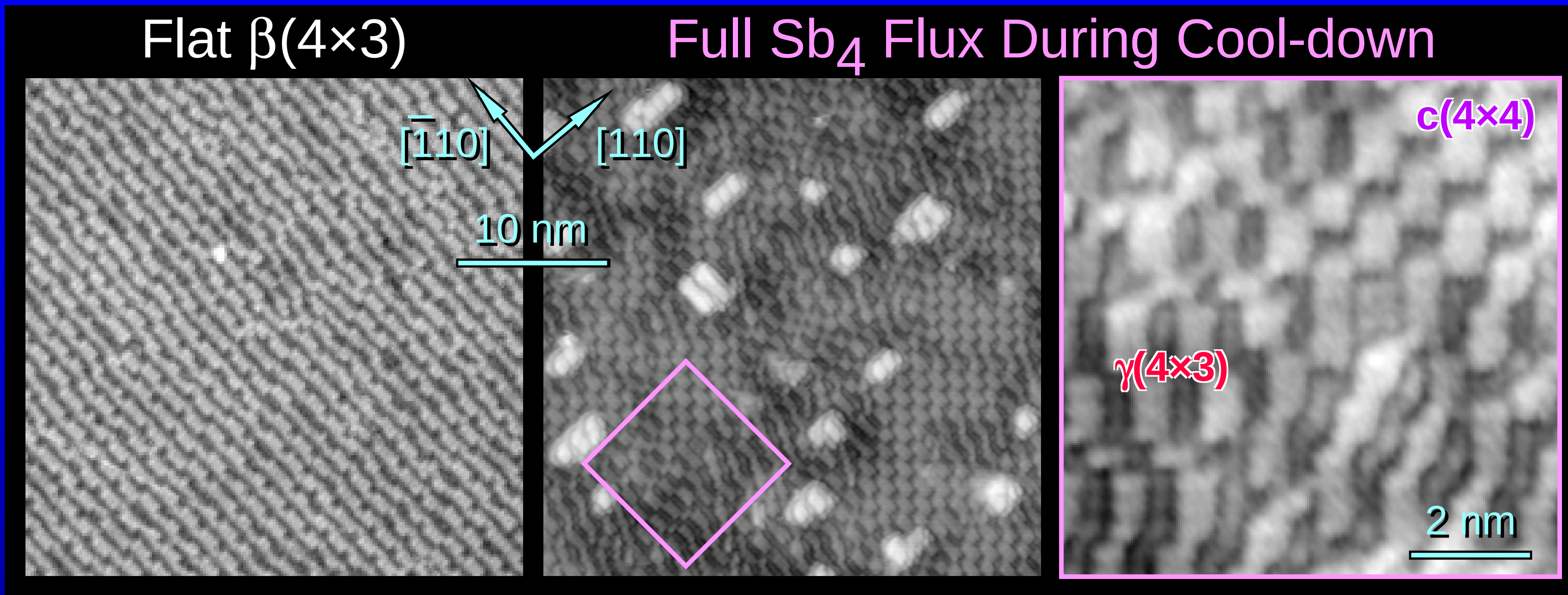
AlSb Island Formation Caused by Reconstruction Change: α-to-β(4×3)



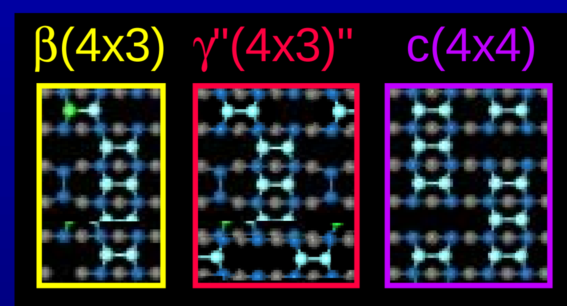
- Converts to α(4×3) during anneal: up to 1/4 ML more Al
- RHEED still "(1×3)"

Restarting growth changes surface back to β(4×3) –> <u>extra islands</u>.

AlSb Island Formation Caused by Reconstruction Change: β-to-γ(4×3)/c(4×4)

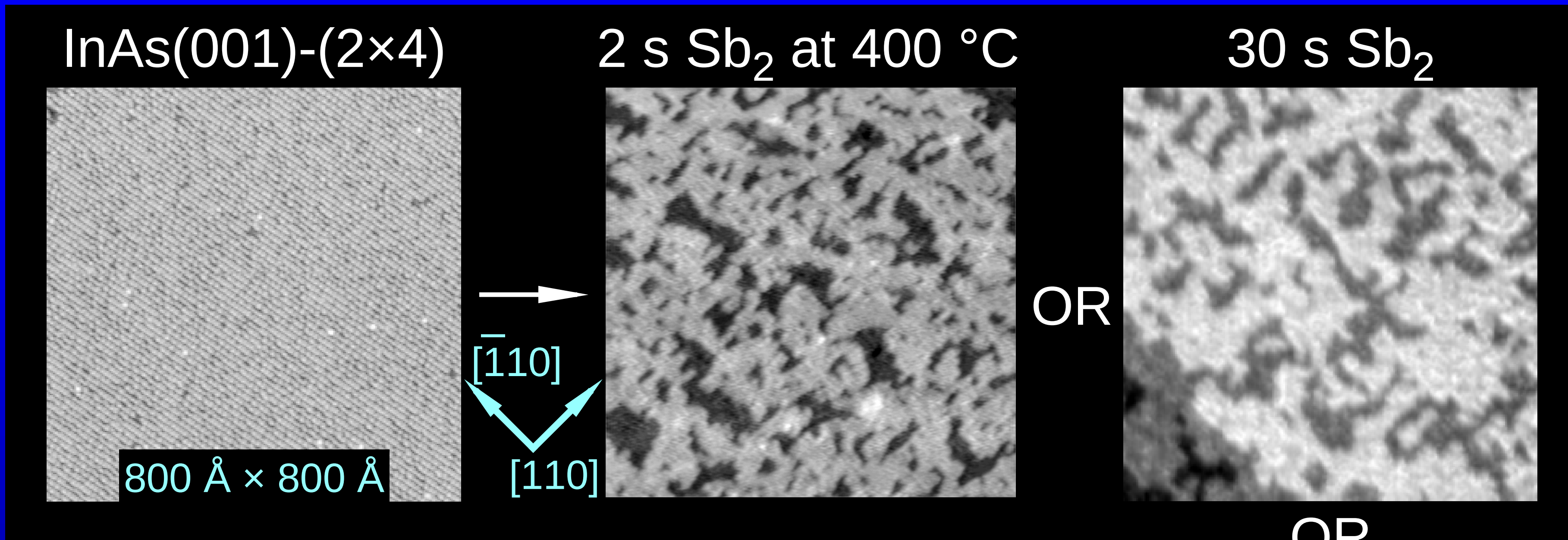


- β(4×3) has 1/12 ML Al on top; γ"(4×3)", c(4×4) only Sb on top
  - RHEED changes to blurry (2×2)+faint 3×
  - <0.1 ML islands created



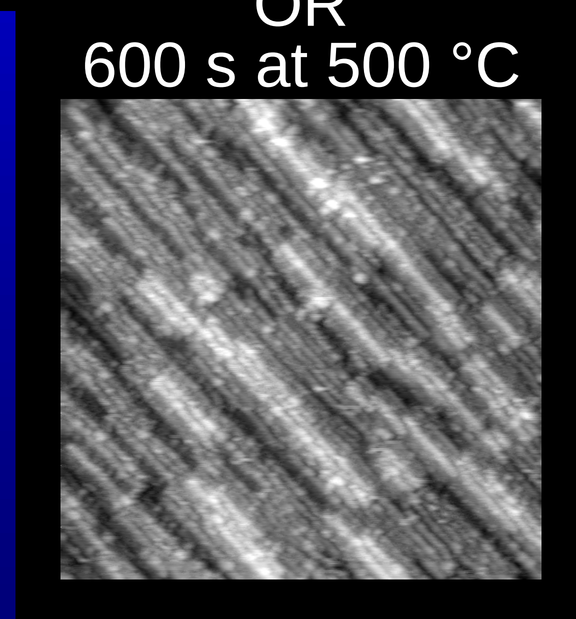
Reconstruction changes are general source of roughness.

Origins of Interfacial Roughness: Sb/InAs

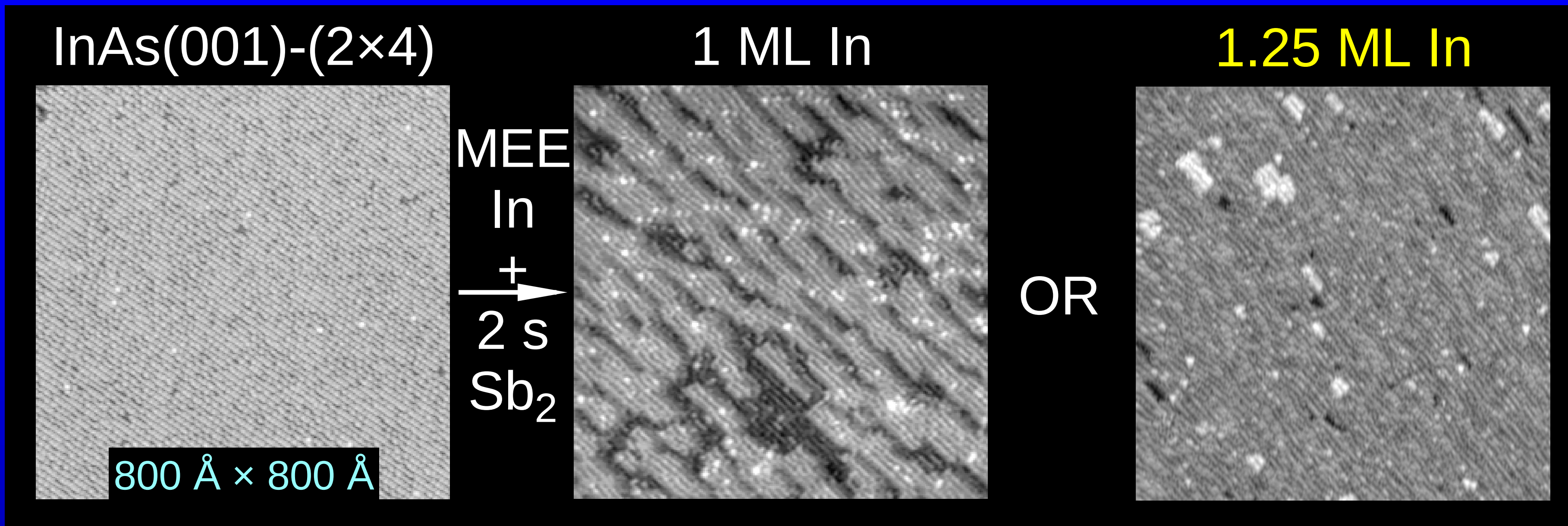


- Sb very reactive: creates 2-level surface with ~25% vacancy islands
- Surface has disordered γ/β(4×3)-like InSb structure

Can NOT anneal out vacancies: get complex reconstruction.

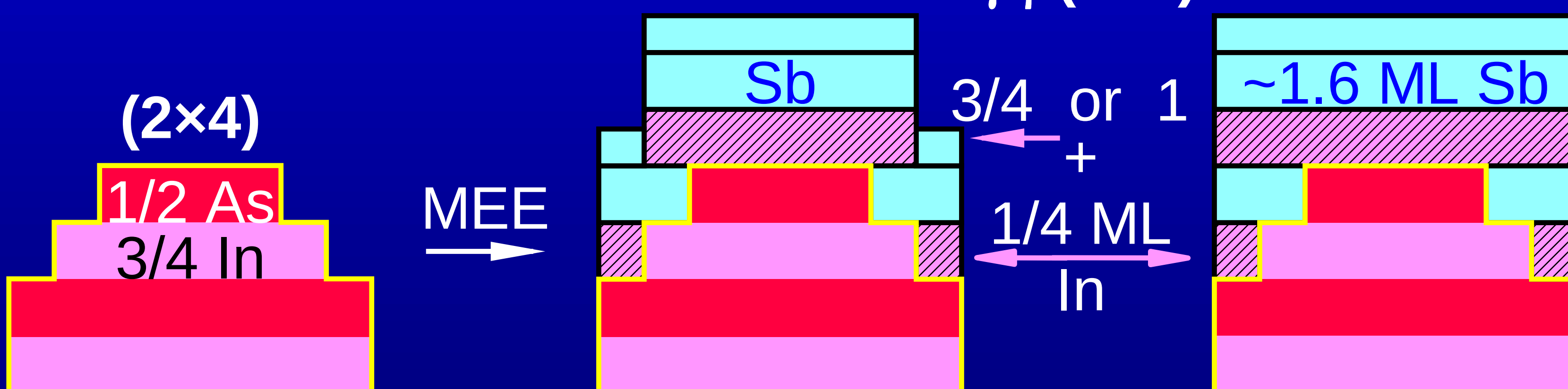


Origins of Interfacial Roughness: Sb/InAs



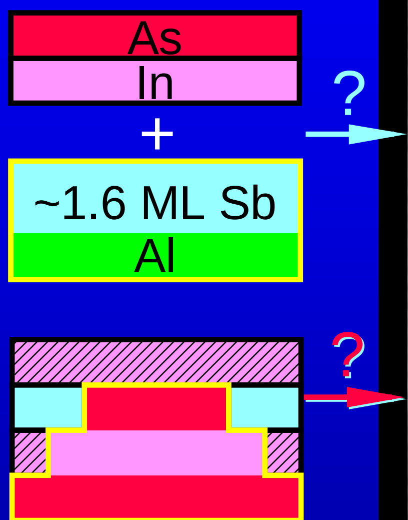
*Nosho, APL **74**, 1704 ('99)*

InSb-like γ/β(4×3) Surfaces

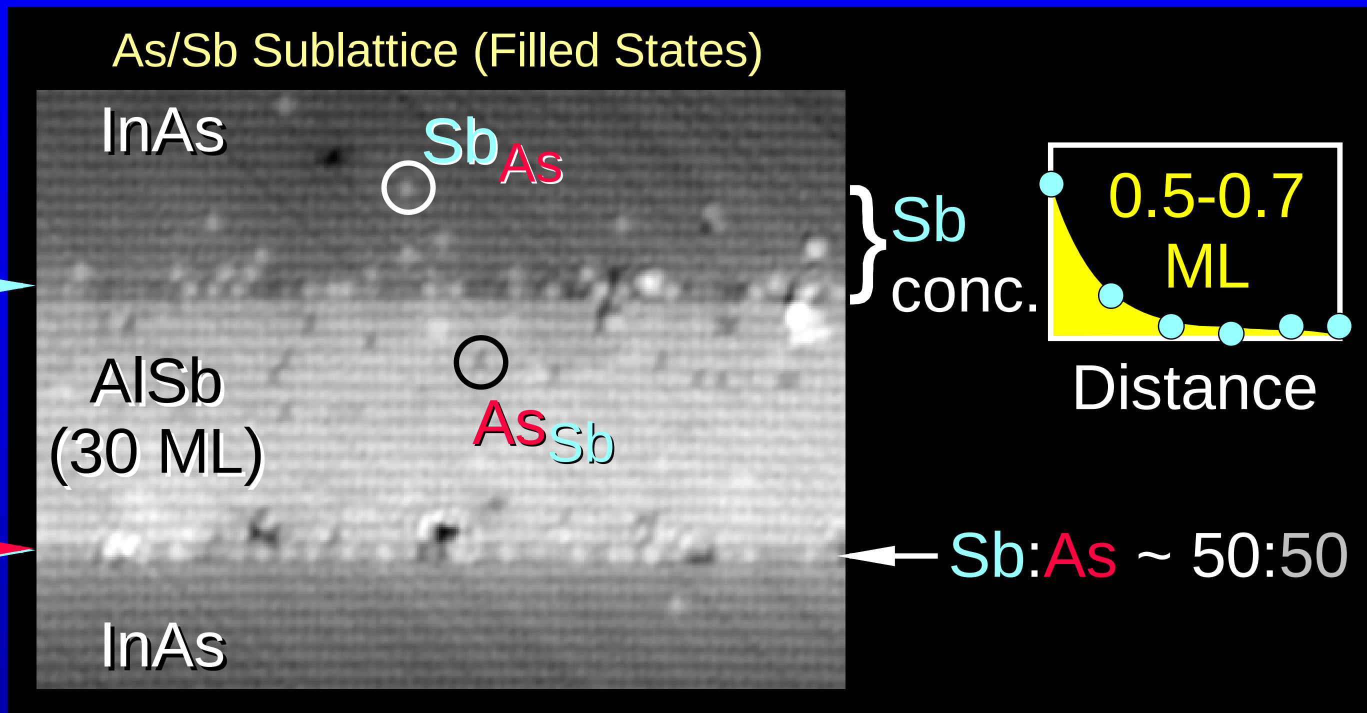


Roughness due to reconstruction stoichiometry again.

AlSb-InAs Interfacial Structure: X-STM



1.25 ML In +
2 s Sb_2

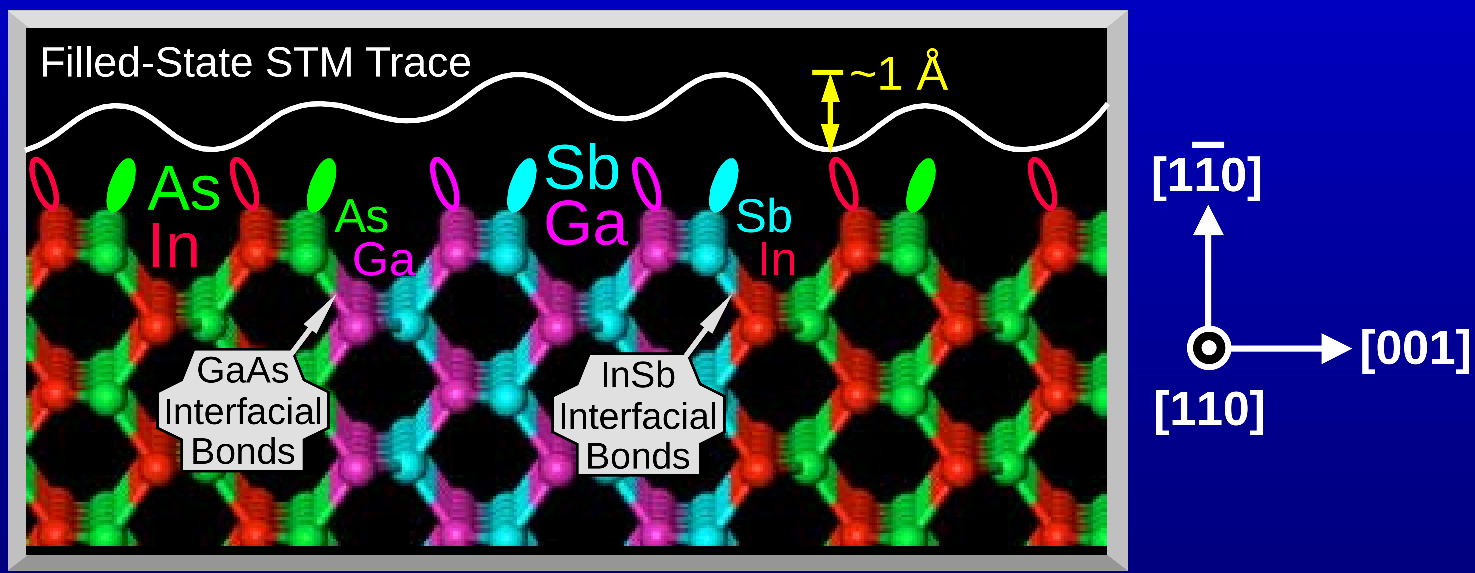


- Looks like original 1/2 ML As remains at AlSb/InAs interface
- Excess Sb from reconstruction floats in InAs/AlSb

X-STM compliments plan-view STM results.

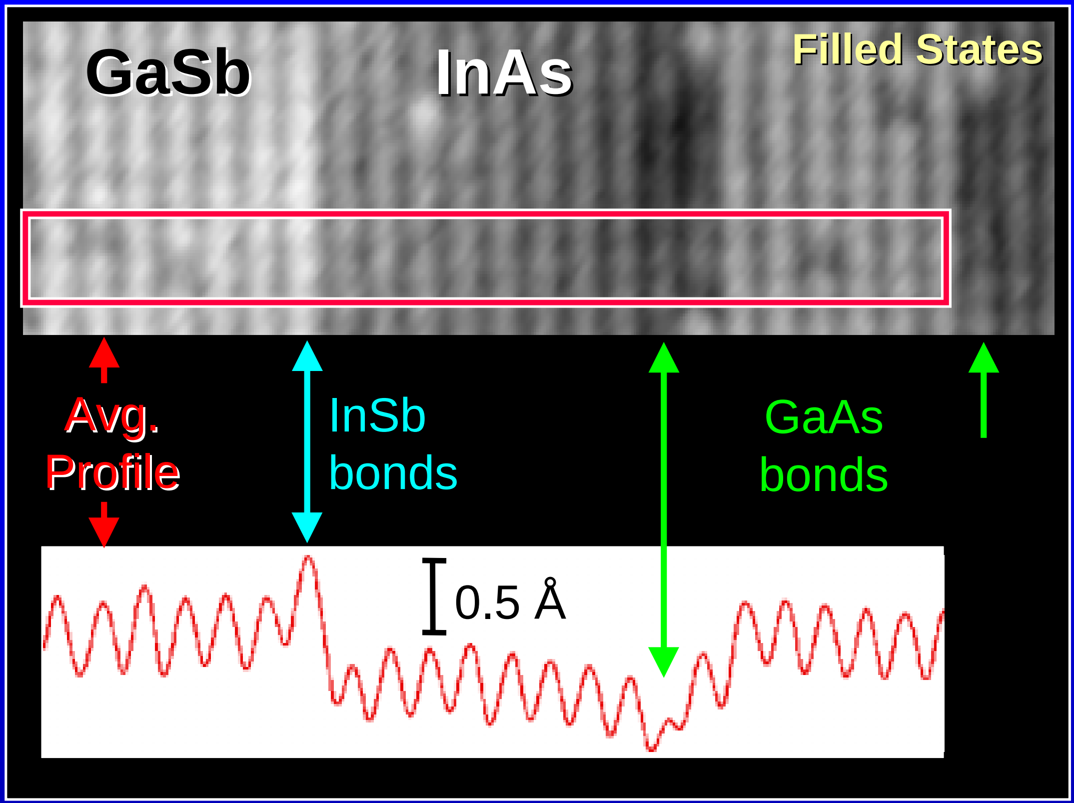
Interpreting X-STM Images

- (110) Surface Structure Artifacts
  - See every-other (001) layer
  - See III **OR** V lattice atoms (bias dependence)
  - Four {110} cleavage faces; e.g. (110) vs. $(1\bar{1}0)$
- Interfacial bond contrast: electronics vs. structural
  - Example: GaAs vs. InSb bonds at InAs-GaSb interface

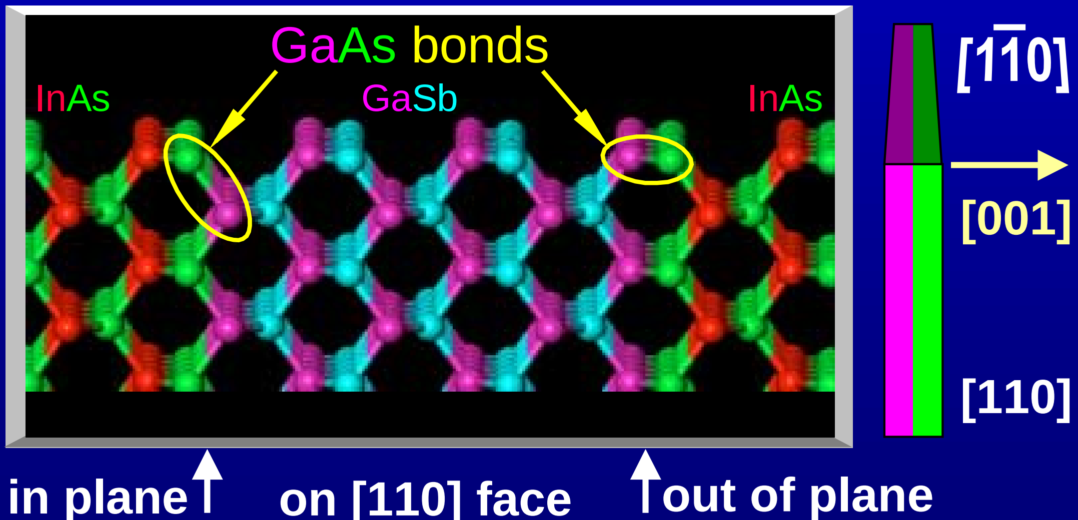


B. Z. Nosho, et al., Surf. Sci. ***465****, 361 (2000)*

Interfacial Bonds in X-STM



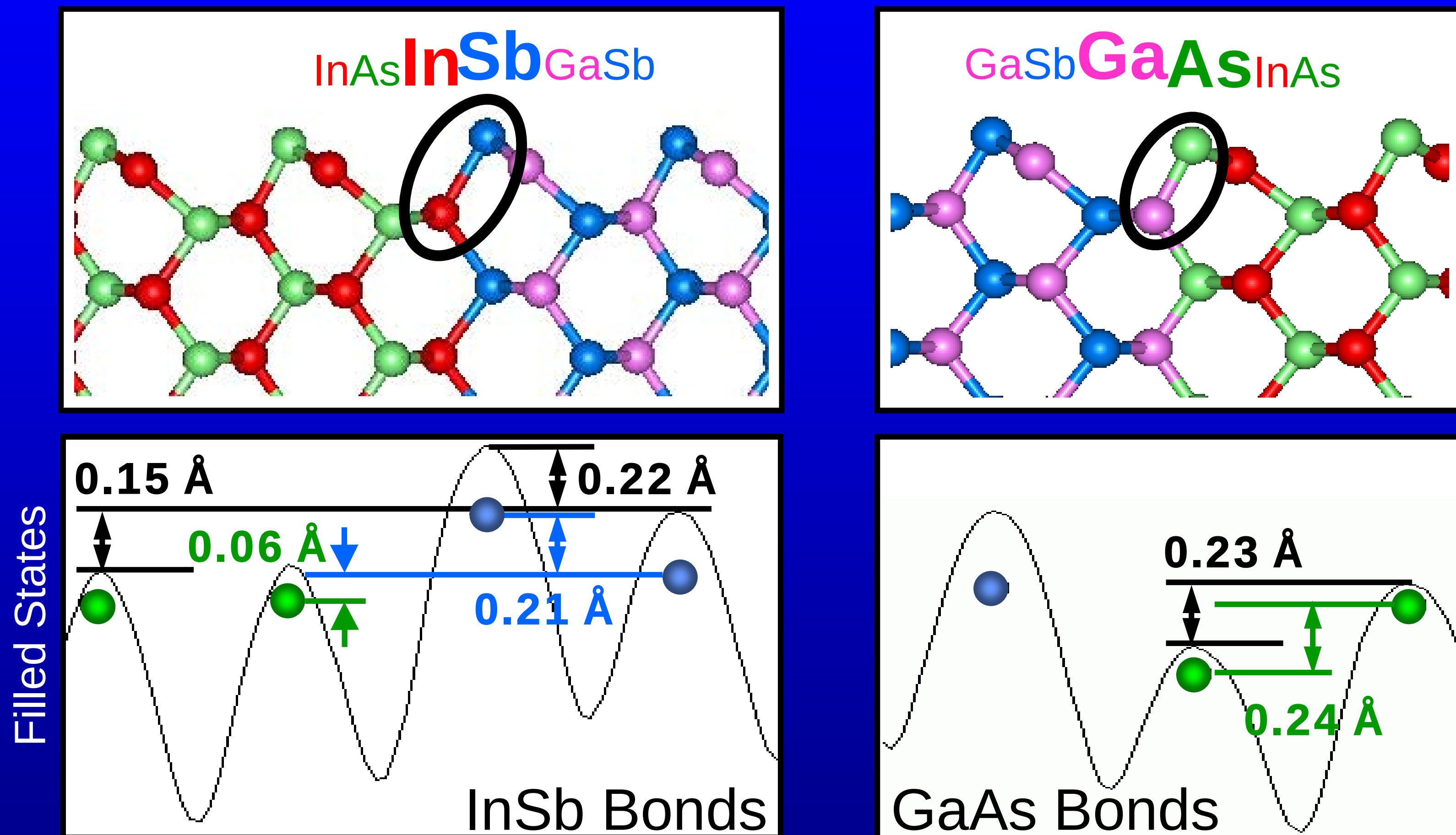
- Only see bond-type contrast at some interfaces
- InSb row higher, GaAs row lower by 0.2-0.3 Å



Bond geometry - in vs. out of plane - depends on cleavage plane and bond type.

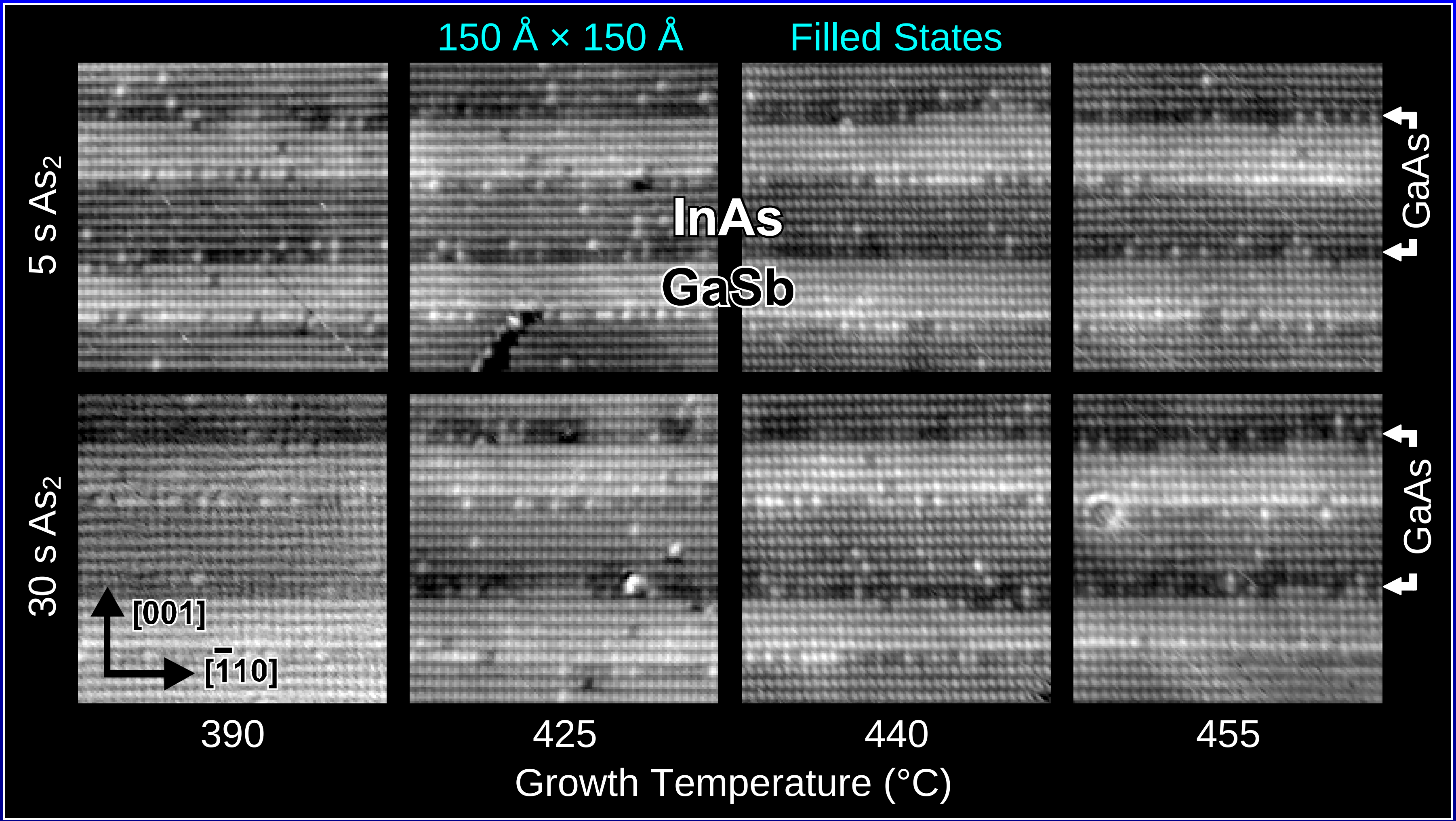
X-STM Contrast from 1st Principles

LDA calculations by S.-G. Kim and S.C. Erwin



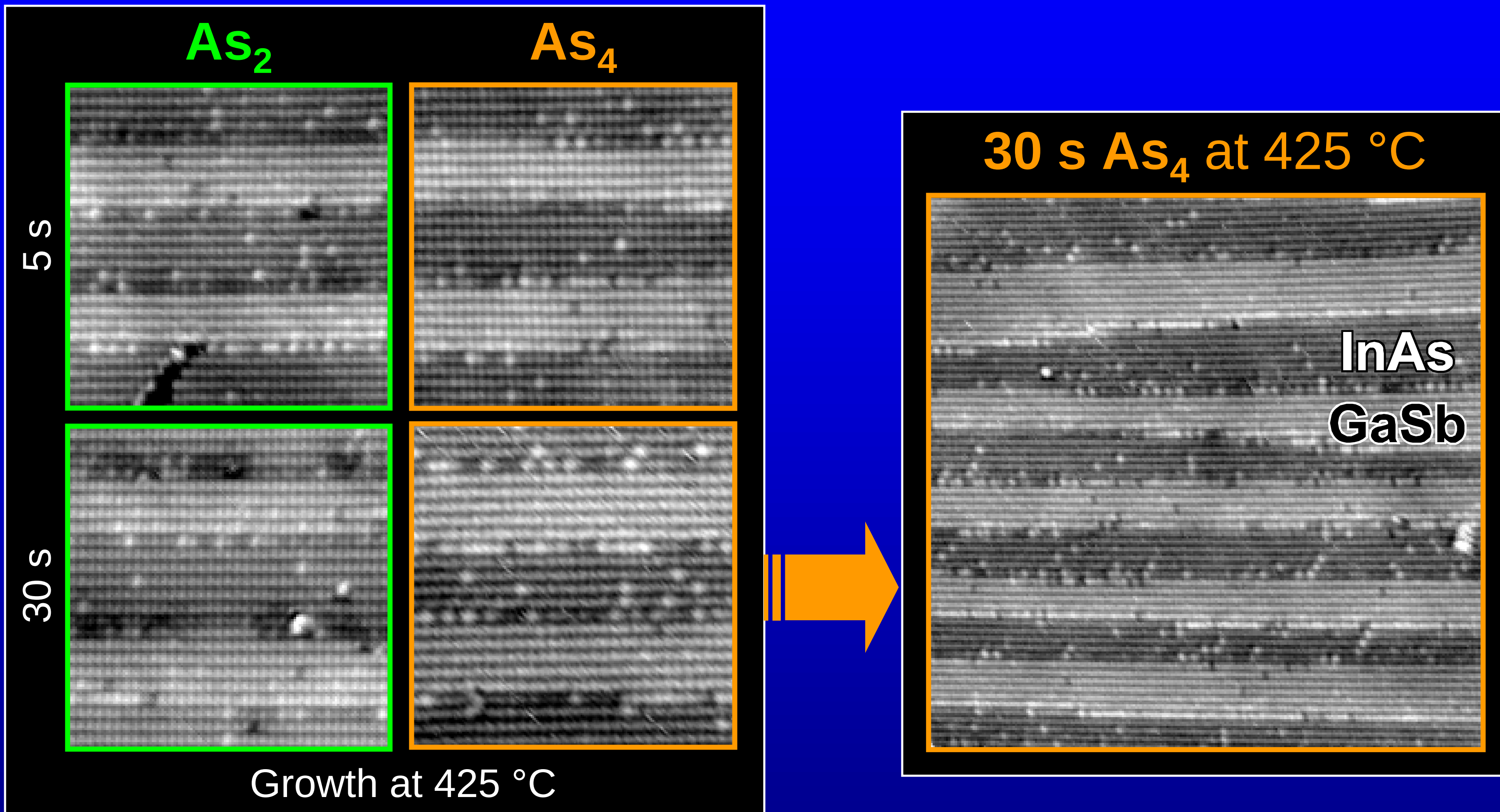
Filled-state contrast: InAs vs. GaSb = 60% *electronic*
Interfacial bonds = 96% *structural*

As_2 Exposures at **InAs/GaSb Interfaces**



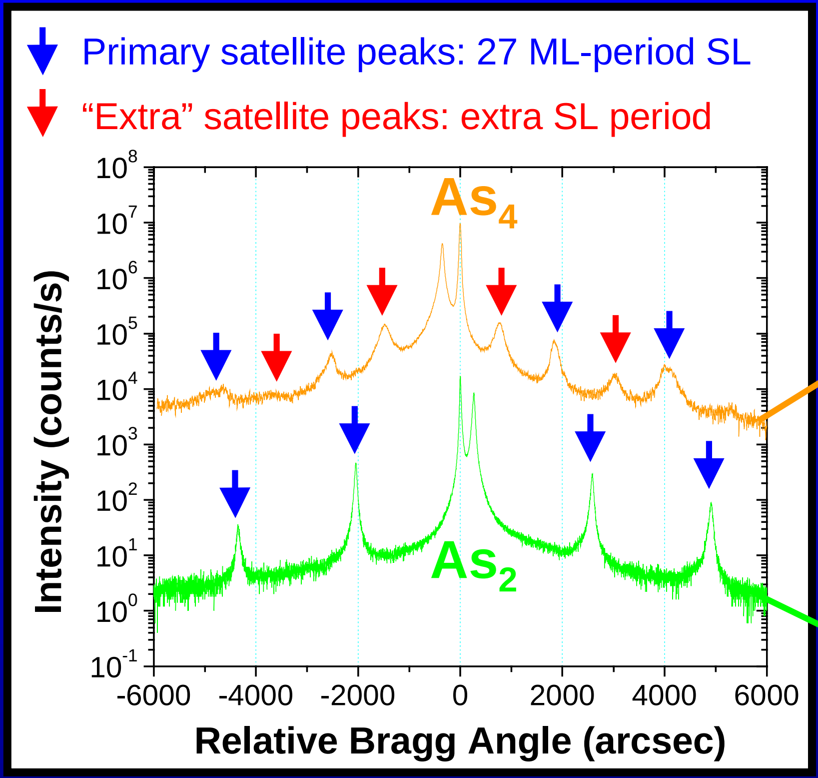
- As_2 on GaSb causes anion exchange rxn ⇒ 1–3 ML GaAs
- Also seen in X-ray diffraction spectra (JVST-B, July 2001)

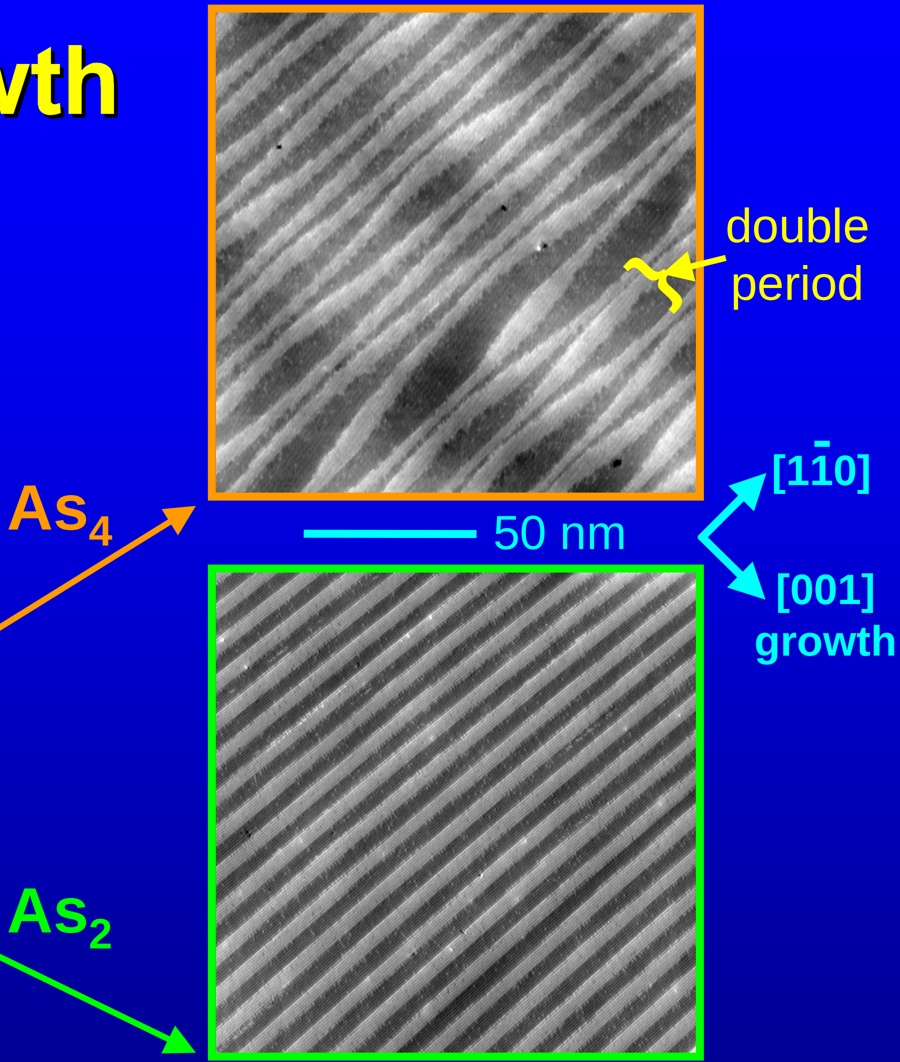
InAs/GaSb Anion Exchange: As_2 vs. As_4



- As_4 causes less GaAs bond formation than As_2
- Somehow degrades superlattice structure

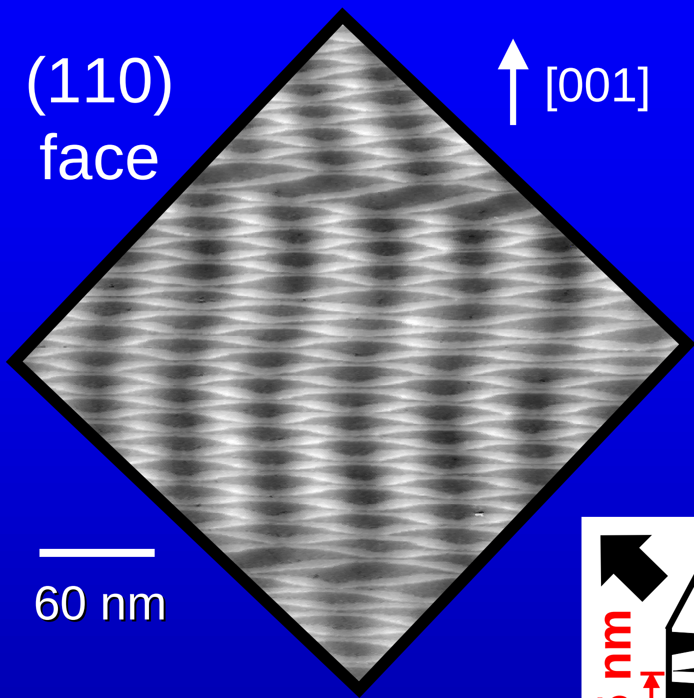
As_4-Induced Growth Instability

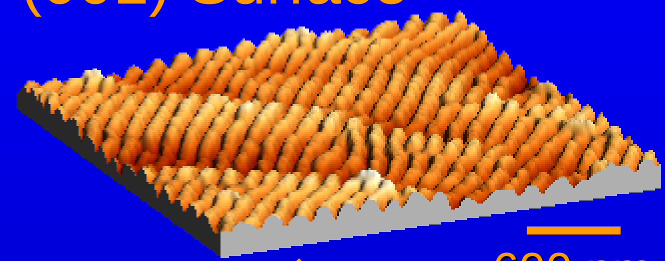


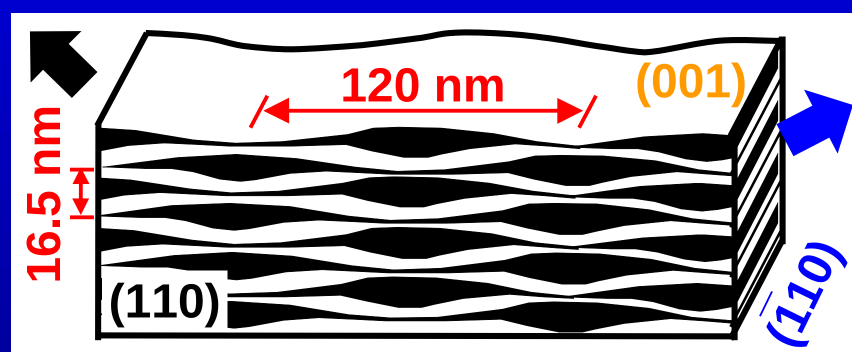


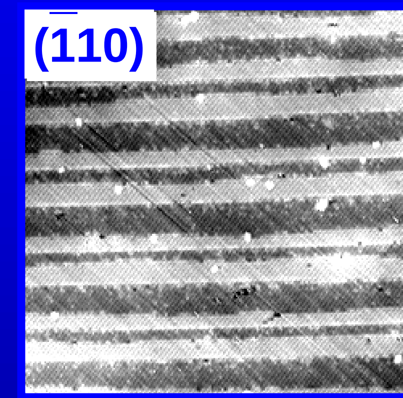
Growth and interrupts with As_4 cause unusual thickness variations w/ period 2x the SL period.

Vertically-Aligned "Quantum Wires"





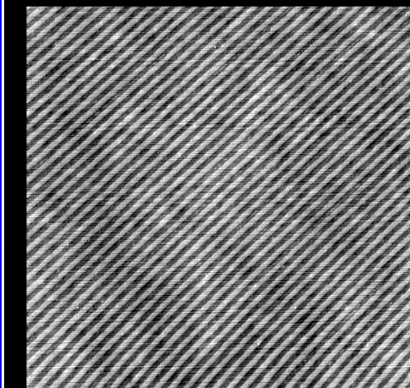
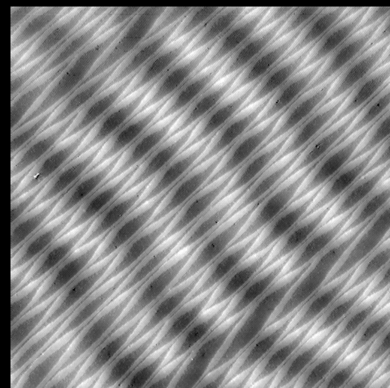
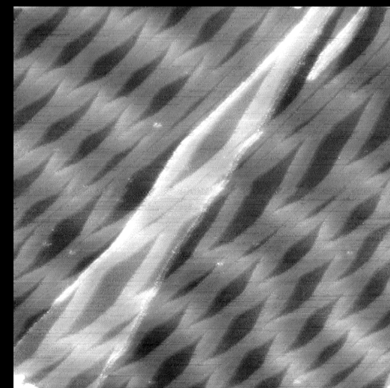
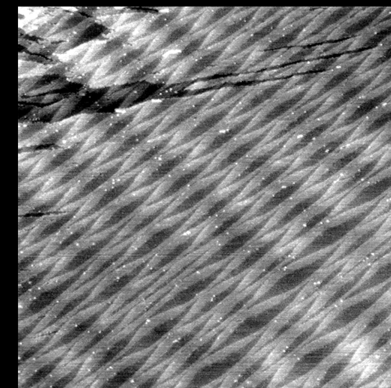




- Vertically-aligned, wire-like structures with long-range order
- 120 nm lateral period, 16.5 nm vertical period
- *Adjacent wires "out-of-phase"*
- Other X-STM contrast from elastic relaxation at {110} surface

Strain Dependence of "Wires"

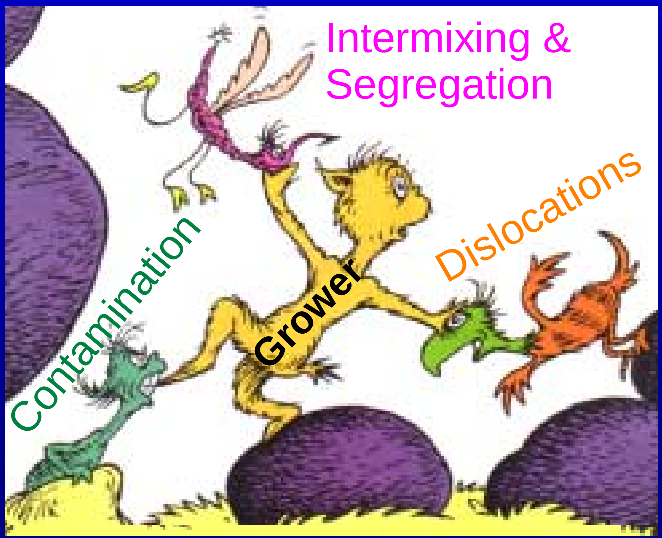
All images 320 nm × 320 nm, (110) face, filled states

InAs Buffer	GaSb Buffer	2xGaSb/GaSb	AlSb Buffer
			
GaSb compressed	GaSb unstrained	GaSb unstrained	GaSb tensile
InAs unstrained	InAs tensile	InAs tensile	InAs more tensile
No Wires!	**τ ~120 nm**	**τ ~150 nm**	**τ ~100 nm**

- Appears to be instability in InAs growth related to strain
- Instability at high As chemical potential (As_4 pressure)
- From HRL (F. Grosse/W. Barvosa-Carter), high As causes:
  - Decreased critical island size $\Rightarrow$ facilitates formation of InAs mounds
  - Anisotropic step formation energies

The Atomic-Scale Structure of Surfaces and Interfaces in III-V Semiconductor Devices

- Understanding of atomic-scale structure critical for surface/interface optimization and modeling
- Surface studies must be integrated with growth effort, device fab., materials characterization, and theory
- Surface vs. material properties: interplay between kinetics and thermodynamics



Next up: Spintronic Devices..

THE END!

Visit us on the web at
http://stm2.nrl.navy.mil/~lwhitman